Glyceryl methacrylate

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Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 3.32e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.34e-01

Confidence level: 3.77e-01

Nearest Neighbors from the Training Set

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1,2-Bis(2-chloroethoxy)ethane

Measured: 1.32e-03 Predicted: 1.34e-01

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Piperazine

Measured: 9.00e-08 Predicted: 7.31e-01

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Dodemorph

Measured: 2.00e-04 Predicted: 6.17e-06

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Cycloheptanone Measured: 2.88e-07 Predicted: 1.00

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Bis(2-chloroethyl) ether Measured: 5.70e-03 Predicted: 3.49